

Biological Computation 20.181

Homework 6

In this homework, you will begin the basic problem of building 3D molecules from an internal reference frame: the rotational angles of each rotatable chemical bond (aka, "torsion space"). However, we will approach these problems from basic geometry.

Building a polymer. We need to determine what information we will need from the chemistry of a molecule to determine its 3D structure. For a 'polymer' of a single atom, there are no real constraints -- we can put the atom anywhere we choose. For simplicity, let's put it at the origin of our reference frame (0,0,0).

If we have two atoms, we can still put the first one at the origin, but the position of the second atom is constrained by the bond length between atoms 1 and 2 (l_{12}). We can choose to place the second atom on the x-axis to keep things simple ($l_{12}, 0, 0$).

For the third atom, we need to consider the bond length to atom 2 (l_{23}) **and** the bond angle formed by atoms 1-3 (a_{123}). We still have some freedom in that we can choose to put these atoms in the x-y plane. If we do so, what will the position of the third atom be?

Write a Python program which returns coordinates for three atoms in the following form:

```
(0, 0, 0)
(?, 0, 0)
(?, ?, ?)
```

given two bond lengths (l_{12} and l_{23}) and one bond angle (a_{123}), which it will read from a file in this format:

```
l12 1.5
l23 1.45
a123 119.5
```

Before the next lecture start to think about what information you will need to place a fourth atom...